

# Cluster virial expansion for nuclear matter within a quasiparticle statistical approach

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Correlations in interacting many-particle systems can lead to the formation of clusters, in particular bound states and resonances. Systematic quantum statistical approaches allow to combine the nuclear statistical equilibrium description (law of mass action) with mean-field concepts. A chemical picture, which treats the clusters as distinct entities, serves as an intuitive concept to treat the low-density limit. Within a generalized Beth-Uhlenbeck approach, the quasiparticle virial expansion is extended to include arbitrary clusters, where special attention must be paid to avoid inconsistencies such as double counting. Correlations are suppressed with increasing density due to Pauli blocking. The contribution of the continuum to the virial coefficients can be reduced by considering clusters explicitly and introducing quasiparticle energies. The cluster-virial expansion for nuclear matter joins known benchmarks at low densities with those near saturation density.

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## I. INTRODUCTION

Recently considerable efforts have been made to elaborate the nuclear matter equation of state (EoS) in a wide range of baryon density  $n$ , temperature  $T$ , and proton fraction  $Y_p$  (or neutron-proton asymmetry  $\delta = 1 - 2Y_p$ ) [1–7]. We consider in this work warm dilute matter ( $T \leq 20$  MeV,  $n \leq n_0$  with  $n_0 \approx 0.16 \text{ fm}^{-3}$  being the nuclear saturation density). In this region the simple model of an ideal Fermi gas of particles has to be improved by including correlations between the particles. It has to be emphasized that the notion of correlations depends on the reference state. For an ideal Fermi gas, the many-body state is given by a Slater determinant of single-particle plane waves without any correlations beyond those originating from quantum statistics. Explicit correlations become less significant near the saturation density because correlations are increasingly blocked with increasing density and Fermi energy and the many-body state can be considered as a system of uncorrelated quasiparticles. At low densities an explicit treatment of correlations is essential. In particular, clusters can dominate the composition of matter at finite density at low temperatures. Different approximations have been considered to treat the formation of clusters in the low-density limit of the nucleon gas, such as the nuclear statistical equilibrium (NSE) approach [6, 8] or virial expansions [9–12]. Here we want to show that a consistent treatment of correlations (bound as well as scattering states) can be given within a quantum statistical approach.

The main question is to match quasiparticle concepts with cluster concepts, as e.g. embodied in the law of mass action at low densities. This has been discussed for the two-nucleon problem within a generalized Beth-Uhlenbeck approach [13] which was developed originally for electron-hole plasmas [14]. A general expression for the second virial coefficient was obtained that contains in addition to the contribution of bound states also those of scattering states. As an important result, it has been demonstrated that the contribution of the continuum of scattering states is modified when quasiparticles are introduced. Larger clusters consisting of  $A$  nucleons were introduced via a cluster decomposition of the nucleon self energy [15]. A quasiparticle treatment of nuclei was considered via an in-medium Schrödinger equation, where, in addition to the single-nucleon self-energy shift, also the Pauli blocking was considered. In-medium quasiparticle energies for the ground states of light nuclei  $A \leq 4$  have been given recently [16] as function of temperature  $T$ , baryon density  $n$ , proton fraction  $Y_p$ , and the center-of-mass momentum  $P$ . The solution of the in-medium few-body problem would also give excited states as well as the scattering states.

Quantum statistical approaches are based on perturbation expansions. Within the Green function method, Feynman diagrams are introduced, and partial summations are performed. We focus on a special prescription to select relevant contributions of the perturbation expansion that describe correctly the formation of clusters in the low-density limit. The concept to include bound states on the same footing as new particle species that can react is called the *chemical picture*. On the other hand, a fundamental quantum statistical approach of interacting elementary particles is the *physical picture*. From this the chemical picture is obtained if in addition to diagrams with single-particle (quasiparticle) propagators also diagrams are considered where the single-particle propagators are replaced by ladder-type

diagrams that describe the propagation of the  $A$  particle cluster. If only the bound state contributions are included, one obtains the NSE in the low-density limit.

If scattering contributions are included in the two-body channel, one obtains the virial expansion. A generalization of the virial expansion is also possible within the chemical picture if in any channel of the cluster-cluster interaction not only the formation of bound states, but also the contribution of scattering states to the thermodynamical properties of the system is considered. Indeed, there are regions in the density-temperature plane where clusters are dominant and should be considered as new constituent particles within the chemical picture. In this case, a cluster-virial expansion should be performed to include the effects of the continuum. Such an approach is evident from the empirical point of view, but not easily derived from first principles. The use of a cluster mean-field (CMF), as well as nearly bound states from the continuum correlations can lead to double counting, and these contributions have to be extracted from the continuum contribution.

Recently, such a cluster-virial expansion has been applied to the proton-neutron- $\alpha$  system [12] and was extended to include additional light clusters [17]. Bound states, such as the deuteron or resonances like  $^8\text{Be}$ , were treated differently, sometimes as part of the generalized second virial coefficient, sometimes as new constituent particles. A systematic derivation of a cluster virial expansion that includes as a limit also the NSE has to be performed on the basis of a fundamental quantum statistical approach. Contributions occurring in higher-order virial coefficients that correspond to bound states or resonances have to be separated since they are explicitly accounted for in the NSE including all nuclei in ground and excited states.

The chemical picture can also be used to derive a cluster-mean field approximation that treats the mean-field effects of a correlated medium [18]. It is expected that the incorporation of mean-field effect into the cluster quasiparticle states will also change the contribution of the scattering states in the cluster-virial expansion. This can be understood from a fundamental point of view by considering the spectral function in the respective  $A$ -nucleon channel. Cluster-quasiparticles should be introduced representing the peaks of the  $A$ -nucleon spectral function. Then the explicit treatment of the contribution of these peaks as quasiparticles will account for a significant part of the total contribution. This is clearly seen in the low-density region where a law of mass action can be introduced. The occurrence of bound states in the EoS according to the law of mass action is a signature that significant contributions have to be extracted from the spectral function of the elementary nucleons. The ordinary quasiparticle picture where the nucleonic spectral function is assumed to be sharply ( $\delta$ -like) peaked is no longer justified.

The inclusion of scattering states is of importance for the equation of state as well as for further properties of nuclear systems. Recently, the composition of low-density nuclear matter was investigated [4] and it was seen in the quantum statistical approach that the contribution of scattering states led to a reduction of the deuteron mass fraction. This has to be taken into account in particular at high temperatures. We will give some details here. The main result is that the contribution of the continuum can be reduced if mean-field and cluster contributions are already extracted.

Some results of the chemical picture are given in Sec. II, however a comprehensive treatment cannot be given here. We discuss the different effects and propose some approximations. The main aim of this paper is to obtain a more systematic treatment in particular of the cluster-virial expansion and to avoid inconsistencies such as double counting. As example, the second virial coefficient is considered in Sec. III that gives the leading contribution in the low density limit. In particular, we discuss the ambiguities connected with the introduction of the bound state contribution of the virial coefficient and the consistent introduction of the quasiparticle picture. The relation to the generating functional approach that allows for a systematic quantum statistical approach to thermodynamic properties is outlined in Sec. IV. Conclusions are drawn in Sec. V, and details are given in the Appendices.

## II. THE CHEMICAL PICTURE AND CORRELATIONS

We explain first some general results for many-particle systems. In the *chemical picture*, we start with a mixture of different constituents that can be the elementary particles (atoms, here nucleons) as well as the bound states (molecules, here nuclei). The main issue is to design approximations where “elementary” particles and “composite” particles are treated on the same footing. This concept has to be incorporated into a quantum statistical approach using Green functions techniques. The cluster Green function approach is briefly summarized in App. A.

### A. Nuclear statistical equilibrium

At low densities we can neglect the interaction with exception of collisions where the constituents come close together resulting in reactions that establish the chemical equilibrium. These reactions include excitations and ionization, e.g., in a plasma. The same considerations apply also for nuclear systems where various nuclei occur that can react. Thus, we have as approximation an ideal mixture of different components.

As a result, the law of mass action is found, with the total particle (baryon) number density (note that astrophysical  $\beta$ -equilibrium is not considered here)

$$n(T, \mu_p, \mu_n) = \sum_{A,Z,\nu} \frac{A}{\Omega} \sum_{\vec{P}} f_A(E_{A,Z,\nu}^{(0)}(\vec{P}), \mu_{A,Z}) \quad (1)$$

where  $A, Z$  denote mass and charge number of a nucleus, respectively, and  $\nu$  indicates the internal quantum state of the nucleus.  $\vec{P}$  is the center of mass momentum,  $\Omega$  is the volume of the system, and

$$f_A(E, \mu) = \frac{1}{\exp[(E - \mu)/T] - (-1)^A} \quad (2)$$

is the Bose or Fermi distribution function for even or odd  $A$ , respectively. Note that at low temperatures Bose-Einstein condensation may occur, which is neglected here. We determine the chemical potentials  $\mu_{A,Z} = Z\mu_p + (A - Z)\mu_n$  only with respect to the kinetic energy of species  $\{A, Z, \nu\}$ , the binding energy  $B_{A,Z,\nu}$  is considered explicitly.

In the low-density limit, the energies

$$E_{A,Z,\nu}^{(0)}(\vec{P}) = -B_{A,Z,\nu} + P^2/(2m_{A,Z,\nu}) \quad (3)$$

are given by the binding energies  $B_{A,Z,\nu}$  of the isolated nuclei in vacuum with masses  $m_{A,Z,\nu} = Zm_p + (A - Z)m_n - B_{A,Z,\nu}$ , denoted by the index (0). In the NSE the summation over  $\nu$  concerns only bound states, the contribution of the continuum is neglected. Neglecting medium corrections, the ordinary law of mass action will increase the mass fraction of bound states like  $d$  and even more the  $\alpha$  particle with respect to the free proton and neutron fractions when the total nucleon number density  $n$  increases. This behavior contradicts the expectation that at high densities a nucleonic quasiparticle picture is appropriate without the explicit occurrence of clusters.

For a more fundamental approach that is not limited to the low-density limit, one should use the *physical picture* where some of the constituents are elementary, while others are composite particles. The composite particles are obtained as bound states of the elementary particles. The same interaction potential, that leads to the formation of bound states in the solution of the many-body Schrödinger equation, determines also the interaction between the constituents of the system. (Note that it is common to formulate statistical physics with 'elementary' particles that on their part are composed of more elementary particles.) The simple law of mass action with clusters where the interaction between the components is neglected (with exception of reactive collisions) works well in the low-density region and low temperatures, in contrast to a picture of an ideal mixture of the elementary particles such as the ideal Fermi gas of protons or neutrons.

## B. Cluster-virial approach

We discuss three issues that are of relevance to improve the NSE. The first one refers to the summation over excited states that, formally, can also be considered as new, independent constituents. Contributions of the continuum are neglected within the chemical picture, and only bound clusters are considered as new 'components'. The limits of this simple chemical picture are evident for sharp resonances above the continuum threshold. Long living states should be included in a more general treatment if the life time (inverse of the width) is sufficiently long. We will consider this problem below within the physical picture using a quantum statistical approach. To obtain the complete second virial coefficient, however, the contribution of scattering states has to be included according to the Beth-Uhlenbeck approach.

The second issue refers to the treatment of the interaction between the different components. The chemical picture takes interactions into account only to establish chemical equilibrium. Effects of scattering correlations on the thermodynamical quantities are neglected. To obtain the full second virial coefficient, the contribution of scattering states has to be included. Nevertheless, the chemical picture describes well the low-density, low-temperature region. It can be improved taking so-called excess terms in the chemical potential and other thermodynamic variables into account. As an example, a simple way to include non-ideal effects is the excluded volume concept [6]. More systematic approaches consider scattering phase shifts due to the interaction between the constituents, as considered in the Beth-Uhlenbeck formula. Then, the total baryon number density

$$n(T, \mu_p, \mu_n) = n_1(T, \mu_p, \mu_n) + n_2(T, \mu_p, \mu_n) + n_3(T, \mu_p, \mu_n) + \dots \quad (4)$$

contains a contribution  $n_1$  from the individual constituents, i.e. nucleons and bound states of nuclei. This term is identical to the NSE result Eq.(1). The contributions  $n_2, n_3, \dots$  account for the two-body, three-body,  $\dots$  correlation

effects in the continuum. In the original Beth-Uhlenbeck formulation there are contributions from bound and scattering two-body correlations appearing in  $n_2$ . However, in order not to count contributions twice as original constituents in  $n_1$  and as bound states in  $n_2$ , the latter term should contain only the scattering part. It can be expressed through integrals with scattering phase shifts  $\delta_c$  in all channels  $c$  for the scattering of nuclei  $\{A, Z, \nu\}$  and  $\{A', Z', \nu'\}$ . Thus it is given by

$$n_2(T, \mu_p, \mu_n) = \sum_{A, Z, \nu} \sum_{A', Z', \nu'} \frac{A + A'}{\Omega} \sum_{\vec{P}} \sum_c g_c \frac{1 + \delta_{A, Z, \nu; A', Z', \nu'}(E)}{2\pi} \int_0^\infty dE f_{A+A'} \left( E_c^{(0)}(\vec{P}) + E, \mu_{A, Z} + \mu_{A', Z'} \right) \frac{d\delta_c}{dE} \quad (5)$$

with energies

$$E_c^{(0)}(\vec{P}) = -B_{A, Z, \nu} - B_{A', Z', \nu'} + \frac{P^2}{2(m_{A, Z, \nu} + m_{A', Z', \nu'})} \quad (6)$$

and degeneracy factors  $g_c$ .

The third issue is related to medium effects. The energies  $E_{A, Z, \nu}^{(0)}(\vec{P})$  and  $E_c^{(0)}(\vec{P})$  in the NSE and the virial expansion, respectively, will be replaced by quasiparticle energies  $E_{A, Z, \nu}(\vec{P}; T, \mu_p, \mu_n)$  of the clusters leading to the generalized cluster Beth-Uhlenbeck approach that is discussed in the next subsection. These quasiparticle energies depend on density and temperature in many-particle systems of finite density. Medium effects become operative if the density exceeds about  $10^{-4} \text{ fm}^{-3}$ . In particular, Pauli blocking will dissolve the clusters at densities about  $10^{-2} \text{ fm}^{-3}$  [16].

The quasiparticle approximation has been used in several recent approaches to calculate the properties of nuclear matter [2, 3, 7]. In particular, it is very effective near saturation density but fails in the low-density region where clusters eventually become of importance. As a first step, we discuss the inclusion of two-particle correlations and the generalized Beth-Uhlenbeck formula, i.e. the  $n_2$  term in Eq.(4), in the following Section. It reproduces the correct second virial coefficient but gives also the correct high-density limit. This allows to reproduce the NSE in the low-density limit but also the transition to the correct behavior in the high-density region.

It will be shown, that both effects, the consideration of the interaction between clusters, i.e. of cluster mean-field effects, as well as the taking into account of excited states and resonances, will reduce the contribution of the continuum to the equation of state, so that appropriate approximations can be obtained.

### C. Generalized cluster Beth-Uhlenbeck approach

Now we discuss the inclusion of medium effects. The effective degrees of freedom are now quasiparticles with self-energies that replace the original constituents. The full evaluation of the imaginary part of the single-nucleon self-energies  $\text{Im } \Sigma_1$  in the so-called  $T_2 G_1$  approximation, see Ref. [13], leads to a generalized Beth-Uhlenbeck equation and corresponding EoS. We can extend this approach, originally formulated with only nucleons as basic constituents, heuristically to consider nucleon and cluster quasiparticles. A systematic treatment based on a generating functional approach is sketched in Section IV.

Considering two-body correlations of nucleons and clusters at most, the total baryon number density

$$n(T, \mu_p, \mu_n) = n_1^{\text{qu}}(T, \mu_p, \mu_n) + n_2^{\text{qu}}(T, \mu_p, \mu_n) \quad (7)$$

receives contributions from single quasiparticles ( $n$ ,  $p$ ,  $d$ ,  $t$ ,  $^3\text{He}$ ,  $^4\text{He}$ , etc.) and correlated two-quasiparticle continuum states. The one-body term

$$n_1^{\text{qu}}(T, \mu_p, \mu_n) = \sum_{A, Z, \nu} \frac{A}{\Omega} \sum_{\substack{\vec{P} \\ P > P_{\text{Mott}}}} f_A(E_{A, Z, \nu}(\vec{P}; T, \mu_p, \mu_n), \mu_{A, Z, \nu}) \quad (8)$$

resembles the corresponding contribution (1) in the NSE and  $n_1(T, \mu_p, \mu_n)$  in the conventional cluster-virial approach discussed in subsections II A and II B. However, there are distinct differences. The quasiparticle energies

$$E_{A, Z, \nu}(\vec{P}; T, \mu_p, \mu_n) = E_{A, Z, \nu}^{(0)}(\vec{P}) + \Delta E_{A, Z, \nu}^{\text{SE}}(\vec{P}; T, \mu_p, \mu_n) \quad (9)$$

depend not only on the c.m. momentum  $\vec{P}$  of the nucleon or cluster with respect to the medium but also on the temperature and chemical potentials (or equivalently densities) through the medium dependent self-energy shift

$\Delta E_{A,Z,\nu}^{\text{SE}}(\vec{P}; T, \mu_p, \mu_n)$ . See App. B and Ref. [16] for a derivation of these shifts. In addition, bound states of clusters exist only for c.m. momenta  $P$  that are larger than the (quasiparticle and medium dependent) Mott momentum  $P_{\text{Mott}}$ . This is mainly a consequence of the Pauli principle that suppresses the formation of clusters due the population of low-momentum states by nucleons of the medium. The Mott momentum  $P_{\text{Mott}}(T, n_n, n_p)$  indicates the critical momentum where the bound state merges with the continuum of scattering states. The Mott momentum becomes larger than zero if the density exceeds a critical value, i.e. above this density bound states can exist only for  $P > P_{\text{Mott}}(T, n_n, n_p)$  [15]. Obviously,  $P_{\text{Mott}} = 0$  for nucleons.

The two-quasiparticle scattering contribution

$$n_2^{\text{qu}}(T, \mu_p, \mu_n) = \sum_{A,Z,\nu} \sum_{A',Z',\nu'} \frac{A+A'}{\Omega} \sum_{\vec{P}} \sum_c g_c \frac{1 + \delta_{A,Z,\nu;A',Z',\nu'}}{2\pi} \times \int_0^\infty dE f_{A+A'} \left( E_c(\vec{P}; T, \mu_p, \mu_n) + E, \mu_{A,Z} + \mu_{A',Z'} \right) 2 \sin^2(\delta_c) \frac{d\delta_c}{dE} \quad (10)$$

is also modified in comparison to the virial result (5) since the energy

$$E_c(\vec{P}; T, \mu_p, \mu_n) = -B_{A,Z,\nu} - B_{A',Z',\nu'} + \frac{P^2}{2(m_{A,Z,\nu} + m_{A',Z',\nu'})} + \Delta E_c^{\text{SE}}(\vec{P}; T, \mu_p, \mu_n) \quad (11)$$

contains the medium-dependent shift  $\Delta E_c^{\text{SE}}(\vec{P}; T, \mu_p, \mu_n)$  of the continuum edge as determined by the the self-energy shifts of the free constituents. Moreover, there is an additional  $2 [\sin(\delta_c)]^2$  factor that reduces the two-body scattering contribution because a part of the two-body correlation effect is shifted to the self-energies of the quasiparticles.

Note that the two-particle contribution (10) describes binary scattering processes  $A, A'$ . A possible bound state contribution in that channel is excluded as contribution to the two-quasiparticle scattering contribution (10). The contribution of a possible  $A + A'$  bound state is already taken into account in the one-body term (8). Thus, double counting is avoided.

### III. COMPARISON OF APPROACHES AT LOW DENSITIES

In the low-density limit, medium effects can be neglected. Only neutrons, protons and deuterons are the relevant constituents. The standard Beth-Uhlenbeck formula for the second virial coefficient and the virial expansion [9, 10] are exact results. They are derived by expanding the thermodynamic functions with respect to the fugacities. It is instructive to show explicitly the equivalence with the generalized cluster Beth-Uhlenbeck approach that introduces the concept of quasiparticles to account for part of the correlations by introducing self-energies.

#### A. Cluster virial approach

Let us first consider the cluster virial method applying a fugacity expansion up to second order in the chemical potentials of protons and neutrons. With the continuum approximation  $(1/\Omega) \sum_{\vec{P}} \rightarrow \int d^3P/(2\pi)^3$  the one-body contribution assumes the form

$$n_1 = n_1^{(p)} + n_1^{(n)} + n_1^{(d)} \quad (12)$$

with the single nucleon contributions ( $i = p, n$ , including degeneracy effects)

$$n_1^{(i)} = \frac{2}{\Lambda_i^3} \left[ \exp\left(\frac{\mu_i}{T}\right) - 2^{-3/2} \exp\left(\frac{2\mu_i}{T}\right) \right] \quad (13)$$

and the single deuteron contribution

$$n_1^{(d)} = \frac{3}{\Lambda_d^3} \exp\left(\frac{\mu_p + \mu_n + B_{2,1}}{T}\right). \quad (14)$$

$\Lambda_i = \sqrt{2\pi/(m_i T)}$  are the thermal wavelengths of the particles  $i = p, n, d$  and  $B_{2,1} > 0$  is the binding energy of the deuteron ground state (identical for all three substates with  $\nu = J_z = -1, 0, 1$ ). The two-body term  $n_2$  in

this approximation is limited to the two-nucleon scattering contributions. Hence, no nucleon-deuteron or deuteron-deuteron correlations are included. In the following, we consider only s-wave contributions for simplicity and have

$$n_2(T, \mu_p, \mu_n) = \frac{2}{\Lambda_p^3} \exp\left(\frac{2\mu_p}{T}\right) b_{pp} + \frac{2}{\Lambda_n^3} \exp\left(\frac{2\mu_n}{T}\right) b_{nn} + \frac{2}{\Lambda_p^{3/2} \Lambda_n^{3/2}} \exp\left(\frac{\mu_p + \mu_n}{T}\right) b_{pn} \quad (15)$$

with the (continuum) virial coefficients (assuming for strong interactions the symmetry  $b_{pp} = b_{nn}$  and  $b_{np} = b_{pn}$ )

$$b_{nn} = 2^{3/2} \int_0^\infty \frac{dE}{\pi} \exp\left(-\frac{E}{T}\right) \frac{d\delta_{1S_0}^{(nn)}}{dE}, \quad (16)$$

$$b_{pn} = 2^{1/2} \int_0^\infty \frac{dE}{\pi} \exp\left(-\frac{E}{T}\right) \left[ \frac{d\delta_{1S_0}^{(pn)}}{dE} + 3 \frac{d\delta_{3S_1}^{(pn)}}{dE} \right] \quad (17)$$

with phase shifts in the isospin triplet ( $T = 1, {}^1S_0$ ) and singlet ( $T = 0, {}^3S_1$ ) channels. The phase shifts can be taken from experiments such that no further model parameters are needed [12]. Instead one can also use for their calculation a nucleon-nucleon interaction potential which is adjusted to describe the empirical scattering phase shifts.

### B. Ambiguity of bound state contributions and physical picture

A partial integration gives the alternative expressions

$$b_{nn} = \frac{2^{3/2}}{T} \int_0^\infty \frac{dE}{\pi} \exp\left(-\frac{E}{T}\right) \delta_{1S_0}^{(nn)}(E), \quad (18)$$

$$b_{pn} = \frac{2^{1/2}}{T} \int_0^\infty \frac{dE}{\pi} \exp\left(-\frac{E}{T}\right) \left[ \delta_{1S_0}^{(pn)}(E) + 3\delta_{3S_1}^{(pn)}(E) \right] - 3\sqrt{2}. \quad (19)$$

for the virial coefficients, since there is the deuteron bound state in the  ${}^3S_1$  channel and the Levinson theorem requires  $\delta_c(0) = n_c\pi$  with the number of bound states  $n_c$  in channel  $c$ . The term  $-3\sqrt{2}$  from the lower boundary of the integral in  $b_{pn}$  can be combined with the bound state contribution  $n_1^{(d)}$  in (12) to give the modified single deuteron contribution ( $\Lambda_d \approx \sqrt{\Lambda_p \Lambda_n / 2}$ )

$$\tilde{n}_1^{(d)} = \frac{3}{\Lambda_d^3} \exp\left(\frac{\mu_p + \mu_n}{T}\right) \left[ \exp\left(\frac{B_{2,1}}{T}\right) - 1 \right]. \quad (20)$$

Both expressions  $n_1^{(d)}$ , Eq. (14) and  $\tilde{n}_1^{(d)}$  (20) are related by a partial integration that changes the contribution of scattering states in the deuteron channel of Eq. (15). Thus we conclude that the contribution of the scattering states can be reduced if the bound state contribution is redefined adequately. Part of the continuum contribution can be transferred to the bound state contribution. Therefore the subdivision of the correlated part of the density into a bound state and a scattering part is ambiguous. This problem has been extensively discussed for Coulomb systems where for the bound state part the Brillouin-Planck-Larkin partition function has been introduced to avoid artificial singularities [19]. As a consequence it makes only sense to consider correlations in a particular channel defined by the corresponding quantum numbers without dividing into bound and scattering parts. Thus we can write

$$n = n_{\text{free}} + n_{\text{corr}} \quad (21)$$

with the contribution of the free nucleons

$$n_{\text{free}} = n_1^{(p)} + n_1^{(n)} \quad (22)$$

and the contribution of the correlated nucleons

$$n_{\text{corr}} = n_1^{(d)} + n_2 = n_{\text{corr}}^{(pp)} + n_{\text{corr}}^{(nn)} + n_{\text{corr}}^{(pn)T=0} + n_{\text{corr}}^{(pn)T=1} \quad (23)$$

that can be split further into the four nucleon-nucleon channels considered above. This point of view corresponds to the *physical picture* where all many-body states are considered as correlations of nucleons.

### C. Continuum correlations and quasiparticle shifts

Coming back to the generalized Beth-Uhlenbeck formula where the single-particle contribution is given by the quasiparticles containing the self-energy shifts, the contribution of the continuum states (10) differs from the simple Beth-Uhlenbeck formula (5). The difference (expressed by the  $2\sin^2(\delta_c)$  term) arises because part of the interaction is already accounted for in the quasiparticle shifts. As shown below in a model calculation, the Born approximation is fully accounted for by the Hartree-Fock (HF) self-energy shifts. Therefore, the introduction of the quasiparticle picture reduces the contribution of the continuum to the virial coefficient. On the other hand, the generalized Beth-Uhlenbeck formula describes the high density region as well where the bound state contributions are suppressed by Pauli blocking.

The lowest order contribution (Born approximation) of the two-body scattering continuum to the EoS can be shifted to the contribution of free quasiparticles with Hartree-Fock mean-field energy shifts. In the physical picture with nucleons as the only degrees of freedom, we start from a non-relativistic Hamiltonian

$$H = \sum_1 E(1)a_1^\dagger a_1 + \frac{1}{2} \sum_{12,1'2'} V(12,1'2')a_1^\dagger a_2^\dagger a_{2'} a_{1'} \quad (24)$$

where  $\{1\}$  denotes the momentum  $\vec{p}_1$ , spin  $\sigma_1$  and isospin  $\tau_1$  characterizing the neutron or proton state. The kinetic energy is  $E(1) = p_1^2/(2m_1)$  and the potential energy contains the matrix element  $V(12,1'2')$  of the nucleon-nucleon interaction. Sophisticated nucleon-nucleon potentials can be used that are fitted to available experimental data. For demonstration, we perform exploratory calculations based on the Yamaguchi separable interaction potential [20],

$$V(12,1'2') = -\frac{\lambda}{\Omega} \frac{\gamma^2}{p^2 + \gamma^2} \frac{\gamma^2}{(p')^2 + \gamma^2} \delta_{P,P'} \delta_{\sigma_2,\sigma_2'} \delta_{\tau_1,\tau_1'} \delta_{\tau_2,\tau_2'} , \quad (25)$$

with the relative momentum  $\vec{p} = (\vec{p}_2 - \vec{p}_1)/2$  and the center-of-mass momentum  $\vec{P} = \vec{p}_1 + \vec{p}_2$  (supposing  $m_p = m_n$ ). Values for the parameters  $\lambda, \gamma$  fitted to nuclear data are given in Ref. [20].

According to the Beth-Uhlenbeck formula, the contribution of the  $nn$  scattering continuum to the density reads (c.f. Eqs. (15) and (16))

$$n_{\text{corr}}^{(nn)} = \frac{2^{5/2}}{\Lambda_n^3} \exp\left(\frac{2\mu_n}{T}\right) \int_0^\infty \frac{dE}{\pi T} \exp\left(-\frac{E}{T}\right) \delta_{1S_0}(E) , \quad (26)$$

where  $E = p^2/m_n$  is the energy of relative motion. For the Yamaguchi potential we have in the weak scattering limit (Born approximation) the phase shift

$$\delta_{1S_0}^{(nn)}(E) = \frac{m_n \lambda \gamma}{4\pi} \frac{\sqrt{\frac{m_n E}{\gamma^2}}}{\left(1 + \frac{m_n E}{\gamma^2}\right)^2} . \quad (27)$$

With this expression we find

$$n_{\text{corr}}^{(nn)} = \frac{2^{3/2}}{\Lambda_n^3} \exp\left(\frac{2\mu_n}{T}\right) \frac{\lambda \gamma^3}{\pi^2 T} \int_0^\infty dx \frac{x^2}{(1+x^2)^2} \exp\left(-\frac{\gamma^2 x^2}{m_n T}\right) \quad (28)$$

by introducing  $x = \sqrt{m_n E}/\gamma$ .

On the other hand, we have from the free quasiparticle contribution in lowest order with respect to  $\lambda$  (Hartree-Fock approximation)

$$n_n^{\text{qu}} = 2 \int \frac{d^3 p_1}{(2\pi)^3} \left[ \exp\left(\frac{p_1^2/(2m_n) + \Delta^{\text{HF}}(p_1) - \mu_n}{T}\right) + 1 \right]^{-1} \quad (29)$$

with the self-energy shift

$$\Delta^{\text{HF}}(p_1) = \sum_{p_2} V(\vec{p}_1 \vec{p}_2, \vec{p}_1 \vec{p}_2)|_{\text{ex}} \left[ \exp\left(\frac{p_2^2/(2m_n) + \Delta^{\text{HF}}(p_2) - \mu_n}{T}\right) + 1 \right]^{-1} . \quad (30)$$

Without the exchange term, that can be neglected at low densities, and after expanding for small  $\Delta^{\text{HF}}$ , we have in the nondegenerate case

$$n_n^{\text{qu}} = 2 \int \frac{d^3 p_1}{(2\pi)^3} \exp\left(-\frac{p_1^2/(2m_n) - \mu_n}{T}\right) \left[1 - \frac{\Delta^{\text{HF}}(p_1)}{T} + \dots\right] = n_1^{(n)} + n_{\text{corr}}^{(nn)} \quad (31)$$

with a term  $n_{\text{corr}}^{(nn)}$  in addition to the free neutron term  $n_1^{(n)}$ . It is given by

$$n_{\text{corr}}^{(nn)} \approx 2 \int \frac{d^3 p_1}{(2\pi)^3} \exp\left(-\frac{p_1^2/(2m_n) - \mu_n}{T}\right) \frac{\Omega}{T} \int \frac{d^3 p_2}{(2\pi)^3} \frac{\lambda}{\Omega} \left[\frac{\gamma^2}{(\vec{p}_2 - \vec{p}_1)^2/4 + \gamma^2}\right]^2 \exp\left(-\frac{p_2^2/(2m_n) - \mu_n}{T}\right). \quad (32)$$

Introducing relative and center-of-mass momenta we have with  $x = p/\gamma$

$$\begin{aligned} n_{\text{corr}}^{(nn)} &\approx 2 \exp\left(\frac{2\mu_n}{T}\right) \int \frac{d^3 P}{(2\pi)^3} \exp\left(-\frac{P^2}{4m_n T}\right) \frac{\lambda}{T} \int \frac{d^3 p}{(2\pi)^3} \left[\frac{\gamma^2}{p^2 + \gamma^2}\right]^2 \exp\left(-\frac{p^2}{m_n T}\right) \\ &= \frac{2^{3/2}}{\Lambda_n^3} \exp\left(\frac{2\mu_n}{T}\right) \frac{\lambda \gamma^3}{\pi^2 T} \int_0^\infty dx \frac{x^2}{(1+x^2)^2} \exp\left(-\frac{\gamma^2 x^2}{m_n T}\right). \end{aligned} \quad (33)$$

The expressions (28) and (33) coincide in the lowest order of the interaction strength  $\lambda$ . The factor  $2[\sin(\delta_{1S_0})]^2$  occurring in the continuum contribution to the density in the generalized Beth-Uhlenbeck formula (10) produces a lowest order  $\mathcal{O}(\lambda^3)$  in the weak interaction limit. Thus, the lower-order contributions in the continuum part of the ordinary Beth-Uhlenbeck formula are transferred to the single quasiparticle term  $n_n^{\text{qu}}$  of the density.

As an example, calculations have been performed for a Yamaguchi interaction fitted to  $nn$  scattering interaction ( $\gamma = 1.3943 \text{ fm}^{-1}$ ,  $\lambda = 704.76 \text{ MeV fm}^3$ ) and for a weaker interaction with half the potential strength, i.e.  $\lambda/2$ , see Fig. 1 with the total baryon number density as a function of the chemical potential  $\mu = \mu_n$  (neutron matter) in different approximations. The correlated part of the density, that is contained in the quasiparticle picture, almost completely reproduces the second virial coefficient in the case of lower interaction strength. For stronger interaction the quasiparticle shift accounts only for a part of the second virial coefficient. Note that the  $nn$  interaction is strong, and the di-neutron is almost bound. Therefore, a mean-field approach is not sufficient to account for the continuum contributions.

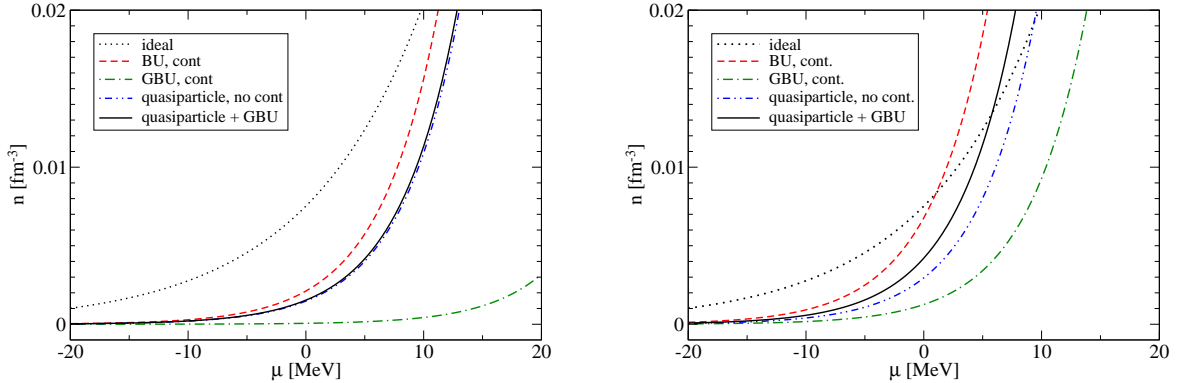


FIG. 1: (Color online) Baryon number density  $n$  as a function of the chemical potential  $\mu$  for  $T = 10 \text{ MeV}$  in neutron matter. Model calculations for a Yamaguchi interaction with an effective range parameter  $\gamma = 1.3943 \text{ fm}^{-1}$  are shown for two values of the coupling strength:  $\lambda = \lambda_0/2$  (left panel) and  $\lambda = \lambda_0$  (right panel), where  $\lambda_0 = 704.76 \text{ MeV}$ . The ideal gas of nucleons (black dotted line) is compared with the correlated part obtained from the standard Beth-Uhlenbeck formula (red dashed line), the generalized Beth-Uhlenbeck formula (green dash-dotted line) containing the factor  $2[\sin \delta]^2$ , the difference in the density if quasiparticles are introduced (blue dash-dotted line), and the total correction part of density (black solid line).

Neutron matter contains no clusters because the interaction is not strong enough to form a bound state. Instead of the cluster virial expansion, we have the standard virial expansion where the second virial coefficient as a benchmark



can be directly related to the observed phase shifts. For details see [5, 21]. The introduction of quasiparticle states and the reduction of the scattering contributions according to the generalized Beth-Uhlenbeck approach [13] is an important issue to go to higher densities.

#### IV. QUANTUM STATISTICAL APPROACH AND THE CLUSTER VIRIAL EXPANSION

A systematic approach to the cluster expansion of thermodynamic properties is obtained from quantum statistics. The grand canonical thermodynamic potential

$$J = -P\Omega = -T \ln \text{Tr} e^{-(H-\mu N)/T}, \quad (34)$$

where  $P$  is the pressure and  $\Omega$  the volume, can be represented by diagrams within a perturbation expansion [22], see also [19]. We have

$$P = \frac{1}{\Omega} \text{Tr} \ln[-G_1^{(0)}] - \frac{1}{2\Omega} \int_0^1 \frac{d\lambda}{\lambda} \text{Tr} \Sigma_\lambda G_\lambda, \quad (35)$$

$$P = P_0 - \frac{1}{2\Omega} \int_0^1 \frac{d\lambda}{\lambda} \left\{ \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} + \text{diagram 5} + \text{diagram 6} + \dots \right\}$$

or

where  $\lambda$  is a scaling factor substituting the interaction  $V$  by  $\lambda V$ .  $G_1^{(0)}$  is the free single-particle propagator that gives

the ideal part of the pressure  $P_0$ . The full single-particle Green function  $G_\lambda$  and the self-energy  $\Sigma_\lambda$  are taken with the coupling constant  $\lambda$ . Depending on the selected diagrams, different approximations can be found. In particular, the second virial coefficient for charged particle systems has been investigated, see Ref. [19]. [41]

An alternative way to derive the equation of state is to start from the expression for the total nucleon density

$$n_{\tau_1}(T, \mu_p, \mu_n) = \frac{2}{\Omega} \sum_1 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f_1(\omega) S_1(1, \omega), \quad (36)$$

where  $\Omega$  is the system volume,  $\tau_1 = n, p$ , and summation over spin direction is collected in the factor 2. Both the Fermi distribution function and the spectral function depend on the temperature and the chemical potentials  $\mu_p, \mu_n$  not given explicitly. The spectral function  $S_1(1, \omega)$  of the single-particle Green function  $G_1(1, iz_\nu)$  is related to the single-particle self-energy  $\Sigma(1, z)$  according to

$$S_1(1, \omega) = \frac{2\text{Im} \Sigma_1(1, \omega - i0)}{(\omega - E(1) - \text{Re} \Sigma_1(1, \omega))^2 + (\text{Im} \Sigma_1(1, \omega - i0))^2}, \quad (37)$$

where the imaginary part has to be taken for a small negative imaginary part in the frequency.

Both approaches are equivalent. As shown by Baym and Kadanoff [22], self-consistent approximations to the one-particle Green function can be given based on a functional  $\Phi$  so that

$$\Sigma_1(1, 1') = \frac{\delta \Phi}{\delta G_1(1, 1')}. \quad (38)$$

Different approximations for the generating functional  $\Phi$  are discussed in the App. D. The self-consistent  $\Phi$ -derivable approximations not only lead to a fully-conserving transport theory. In the equilibrium case they also have the property that different methods to obtain the grand partition function such as integrating the expectation value of the potential energy with respect to the coupling constant  $\lambda$ , or integrating the density  $n$  with respect to the chemical potential  $\mu$ , lead to the same result. In particular, with

$$J = -\text{Tr} \ln(-G_1) - \text{Tr} \Sigma_1 G_1 + \Phi \quad (39)$$

also

$$n = -\frac{1}{\Omega} \frac{\partial J}{\partial \mu} \quad (40)$$

holds in the considered approximation.

The latter approach using Eq. (36) has been extensively used in many-particle systems [13–15], in particular in connection with the chemical picture. An analysis of the self-energy allows to work out a diagram technique that treats bound states on the same footing as “elementary” single particle described by the free propagator

$$G_1^{(0)}(1, z) = \frac{1}{z - E_1(p_1)}. \quad (41)$$

Considering the  $A$ -particle propagator (A6) in the low-density limit where we can drop all medium effects, the solution of the Bethe-Salpeter equation in ladder approximation gives the propagator for the  $A$ -particle bound states

$$G_{A,\nu}^{\text{bound}}(1 \dots A; 1' \dots A'; z_A) = \langle 1 \dots A | \psi_{A\nu P} \rangle \frac{1}{z_A - E_{A,\nu}^{(0)}(P)} \langle \psi_{A\nu P} | 1' \dots A' \rangle \quad (42)$$

where  $\nu$  indicates the internal quantum state of the  $A$ -particle bound state, after separation of the center-of-mass momentum  $\vec{P}$ . As a new element, the bound state propagator is introduced as indicated in Fig. 2. This bound state propagator has the same analytical form like the single particle propagator (41), besides the appearance of the internal wave function that determines the vertex function.

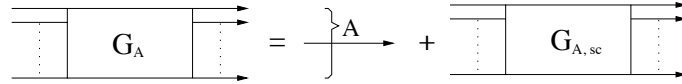


FIG. 2: Splitting of the  $A$ -particle cluster propagator into a bound and scattering contribution. Note that the internal quantum number has been dropped.

As example, in App. D different approximations are obtained such as the nuclear statistical equilibrium (NSE) and the cluster mean-field (CMF) approximation using the chemical picture. These approximations are based on the bound state part of the  $A$ -particle propagator. They give leading contributions in the low-density, low temperature range where bound states dominate the composition of the many-particle system. From the point of view of the physical picture, these contributions arise in higher orders of the virial expansion of the equation of state. As example, the formation of the  $A$ -particle bound state is seen in the  $A$ -th virial coefficient, the mean-field shift due to a cluster  $B$  in the  $(A + B)$ -th virial coefficient. The chemical picture indicates which high-order virial coefficients of the virial expansion are essential, if the many-particle system is strongly correlated so that bound states are formed.

As an example, Hydrogen molecules dominate the electron-proton system under normal conditions. The effective interaction can be calculated, and the corresponding virial coefficient determines the non-ideal part of the Hydrogen EoS. Local effective interactions are the Lennard-Jones or the Morse potential, and the Mayer cluster expansion can be used to evaluate the Hydrogen-Hydrogen virial coefficient. Within the physical picture based on electrons and protons, the eighth-order virial coefficient has to be analyzed to find the non-ideal features of the Hydrogen gas. Similar approaches can also be used for  $\alpha$  matter in nuclear physics, introducing effective interactions such as the Ali-Bodmer potential.

Using the quasiparticle approach, the EoS, Eq. (8), is obtained, see App. A. In contrast to the NSE, Eq. (1), medium dependent quasiparticle energies are used. In the cluster mean-field (CMF) approximation only the first-order terms of the cluster-cluster interaction are taken into account. The remaining part of the continuum correlations is neglected.

To improve the approximation, the scattering part of the  $A$ -particle propagator has to be considered. It contributes also to the  $A$ -th virial coefficient. The scattering processes within the  $A$ -particle system can have different channels. As an example we discuss here binary elastic scattering processes between sub-clusters  $A_1$  and  $A_2$  of the system of  $A$  particles,  $A = A_1 + A_2$ . Binary phase shifts  $\delta_{A_1, A_2}(E)$  are introduced that describe the corresponding scattering experiments. They can also be calculated within few-body theory. Besides the effective interaction between the sub-clusters that are depending on the internal wave function of the sub-clusters, also virtual transitions to excited states have to be taken into account. In general, the effective interaction is non-local in space and time, i.e. momentum and frequency dependent.

The generalized cluster Beth-Uhlenbeck formula (10) is obtained when in particle loops not the free propagator, but quasiparticle Green's functions are used. If the quasiparticle shift is calculated in Hartree-Fock approximation, the first order term of the interaction must be excluded from the ladder  $T_2^{\text{ladder}}$  matrix to avoid double counting. The bound state part is not affected, it is determined by an infinite number of diagrams. The scattering part is reduced subtracting the Born contribution as shown in Eq. (10) by the  $2[\sin(\delta_c)]^2$  term; for the derivation see Ref. [13].

The continuum correlations that are not considered in the NSE give a contribution to the second virial coefficient in the chemical picture. We can extract from the continuum part two contributions: resonances that can be treated

like new particles in the law of mass action, and the quasiparticle shift of the different components contributing to the law of mass action. Both processes are expected to represent significant contributions of the continuum. After projecting out these effects, the residual contribution of the two-nucleon continuum is assumed to be reduced. One can try to parametrize the residual part, using the ambiguity in defining the bound state contribution, see Sec. III B. Eventually the residual part of the continuum correlations can be neglected.

## V. CONCLUSIONS

We have shown that it is possible to give a unified description for the nuclear matter equation of state that joins the region of saturation density, where quasiparticle approaches can be used, with the low-density region where the Nuclear Statistical Equilibrium or, more rigorously, the virial expansion can be applied. The chemical picture that allows for a systematic treatment of all bound states is used as guide line to formulate cluster expansions of different quantities such as self-energy, density and pressure. The inclusion of arbitrary nuclei as demanded by the chemical picture is indispensable to derive the nuclear matter EoS.

As a main ingredient, the generalized Beth-Uhlenbeck formula [13, 15] that treats the two-particle correlations already joins the low-density limit with the saturation density region. It is extended to clusters with arbitrary mass number [15] and has been investigated recently [4] to derive the thermodynamic properties of nuclear matter in the subsaturation density region.

Whereas the bound states are treated in a systematic way, the continuum of scattering states needs further investigations, especially if many channels appear in the continuum. The approach presented is to extract important contributions from the continuum that are of relevance for the physical properties. We discussed three contributions: i) Resonances in the continuum can be considered similar to bound states. As example, we can consider  $A = 8$  and the subdivision into two  $\alpha$  particle clusters. The  $\alpha - \alpha$  elastic scattering phase shifts can be used to find a contribution to the corresponding cluster-virial coefficient.  ${}^8\text{Be}$  as a sharp resonance can be treated as new particle in the chemical picture and should be projected out from the scattering contribution to the equation of state.

ii) Mean-field effects can be extracted introducing quasiparticles not only for the single nucleon states, but also for the bound states. This reduces the interaction contribution to the continuum states. We have shown that in the weak scattering limit the continuum contributions are transferred to the quasiparticle energy shifts. In particular, the generalized Beth-Uhlenbeck formula shows this behavior.

iii) There is no first principle distinction between the contribution of bound states and scattering states to the virial coefficient. For instance, partial integration and using the Levinson theorem gives different expressions for the contribution of bound states, see Sec. III B. The contribution of the bound states to the virial coefficient is not unambiguously defined. This allows to find optimal approximations to take the contribution of the continuum into account.

In conclusion, the cluster-virial expansion in combination with the consideration of excited states, resonances, and the introduction of the quasiparticle concept allows to extract relevant contributions from the continuum states. The remaining contributions of the continuum of the cluster-virial coefficients can be included into the sum over the internal quantum number  $\nu$  in the respective cluster-cluster channel. A systematic approach to the residual contribution that avoids double-counting is possible starting from the generating functional, but needs further study including investigations of topological aspects to characterize sets of relevant diagrams within the perturbation expansion. This is a complex problem and has to be worked out in future. Alternatively one can also use numerical methods to simulate the many-nucleon systems in the intermediate region. This way the interpolation between the saturation density and the low-density limit can be improved.

Improved calculations of the nuclear matter EoS take the contribution of the continuum to the second virial coefficient into account. The ambiguity in the definition of the bound state contribution has been used in quantum statistical calculations, see the quantum statistical calculation in Ref. [4] and the recent work [5]. Formally, the summation over the internal quantum number  $\nu$  can be used to consider also the contribution of scattering states, as well-known from the Planck-Larkin partition function in plasma physics [19]. The effect of the correct treatment of continuum correlations for calculating the composition of nuclear matter is shown in Ref. [4]. The dissolution of clusters with increasing density was calculated within two different approaches, the quantum statistical approach where the second virial coefficient was taken into account, and the generalized RMF approach where continuum contributions are neglected. The largest discrepancies are obtained for the deuteron fraction at high temperatures when the deuteron binding energy is small compared with the temperature (see also [5]). The influence of the correct treatment of continuum correlations in the deuteron channel on other thermodynamic quantities can also be seen when comparing both approaches. The systematic inclusion of further scattering phase shifts, e.g., in the  $\alpha - \alpha$  channel, within the cluster virial expansion would give an improved approach to all thermodynamic quantities.

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### Appendix A: Cluster expansion of the single-nucleon self-energy

To include nuclei with arbitrary mass number  $A$ , a cluster decomposition of the single-nucleon self-energy can be performed [15]. In particular, the inclusion of the light elements  ${}^3\text{H}$ ,  ${}^3\text{He}$ , and  ${}^4\text{He}$  has been discussed in [4]. We will not repeat the Green function approach here, see, e.g., Refs. [4, 15, 16] but give only some final results. The nucleon density is expressed in terms of the spectral function. The latter is related to the single-nucleon self-energy that is represented by Feynman diagrams. According to the chemical picture, the single nucleon propagators that occur in the self-energy have to be replaced by propagators of arbitrary clusters. The cluster decomposition of the self-energy yields the law of mass action and the NSE. The mean-field approximation has to be replaced by a cluster mean-field approximation as given in App. B. This way the quasiparticle concept for the single-nucleon state is extended to arbitrary clusters.

The evaluation of the self-energy gives

$$\Sigma(1, z_\nu) = \sum_A \sum_{z_A, 2 \dots A} G_{(A-1)}^{(0)}(2, \dots, A, iz_A - iz_\nu) T_A(1 \dots A, 1' \dots A', z_A) \quad (\text{A1})$$

with the free  $(A-1)$  (quasi-) particle propagator

$$G_{(A-1)}^{(0)}(2, \dots, A, z) = \frac{1}{z - E_2 - \dots - E_A} \frac{f_{1, z_2}(2) \dots f_{1, z_A}(A)}{f_{A-1, z_{A-1}}(E_2 + \dots + E_A)}. \quad (\text{A2})$$

The quantity  $z_\nu$  is the single-particle Matsubara frequency, and  $z_A$  that of the  $A$ -particle system. The  $A$ -particle  $T$  matrix is obtained from the  $A$ -particle Green function by amputation.

The  $A$ -particle Green function obeys in ladder approximation a Bethe-Salpeter equation (BSE)

$$\begin{aligned} G_A(1 \dots A, 1' \dots A', z_A) &= G_A^{(0)}(1 \dots A, z_A) \delta_{11'} \dots \delta_{AA'} \\ &+ \sum_{1'' \dots A''} G_A^{(0)}(1 \dots A, z_A) V^{A, \text{mf}}(1 \dots A, 1'' \dots A'') G_A(1'' \dots A'', 1' \dots A', z_A) \end{aligned} \quad (\text{A3})$$

where  $V^{A, \text{mf}}(1 \dots A, 1' \dots A') = \sum_{i < j} [V_{ij} + \Delta V_{ij}^A]$  is the interaction within the  $A$ -particle cluster, including mean-field contributions, see App. B. The free  $A$ -quasiparticle Green function results as

$$G_A^{(0)}(1 \dots A, z_A) = \frac{[1 - \tilde{f}_1(1)] \dots [1 - \tilde{f}_1(A)] - \tilde{f}_1(1) \dots \tilde{f}_1(A)}{z_A - E_1^{\text{qu}}(1) - \dots - E_1^{\text{qu}}(A)}. \quad (\text{A4})$$

The approximation of an uncorrelated medium, see App. C, leads to the effective occupation numbers

$$\tilde{f}_1(1) = \frac{1}{\exp[E_1^{\text{qu}}(1)/T - \tilde{\mu}_\tau/T] + 1} \approx \frac{n_\tau}{2} \left( \frac{2\pi\hbar^2}{mT} \right)^{3/2} e^{-E_1^{\text{qu}}(1)/T} \quad (\text{A5})$$

in the low-density, non-degenerate limit ( $\tilde{\mu}_\tau < 0$ ), where  $\tilde{\mu}_\tau$  is determined by the normalization condition  $2 \sum_p \tilde{f}_1(p) = n_\tau$ , where  $\tau$  denotes isospin (proton or neutron).

The solution of the BSE is given by an expansion, bilinear in the wave functions

$$G_A(1 \dots A, 1' \dots A', z_A) = \sum_{\nu P} \psi_{A\nu P}(1 \dots A) \frac{1}{z_A - E_{A\nu P}^{\text{qu}}} \psi_{A\nu P}^*(1' \dots A'). \quad (\text{A6})$$

The summation over the internal quantum states  $\nu$  includes besides the bound states also the scattering states. The  $A$ -particle wave function and the corresponding eigenvalues follow from solving the in-medium Schrödinger equation

$$[E_1^{\text{qu}}(1) + \dots + E_1^{\text{qu}}(A) - E_{A\nu}^{\text{qu}}(P)]\psi_{A\nu P}(1 \dots, k, \dots A) + \sum_{1' \dots A'} \sum_{i < j} [1 - \tilde{f}_1(i) - \tilde{f}_1(j)] V(ij, i'j') \prod_{k \neq i, j} \delta_{kk'} \psi_{A\nu P}(1' \dots, k', \dots A') = 0. \quad (\text{A7})$$

This equation contains the effects of the medium in the quasiparticle shift as well as in the Pauli blocking terms. Obviously the bound state wave functions and energy eigenvalues as well as the scattering phase shifts become dependent on the c.m. momentum  $P$ , temperature  $T$ , and densities  $n_p, n_n$ .

Two effects have to be considered, the quasiparticle energy shift and the Pauli blocking. Detailed results have been obtained for the two-nucleon case. The shift of the binding energy and the medium modification of the scattering phase shifts are discussed extensively, see [13, 40]. The solutions of the in-medium Schrödinger equation (A7) for  $A = 2, 3, 4$  was parametrized recently [16].

## Appendix B: The Cluster-mean field (CMF) approximation

The chemical picture gives the motivation to extend the mean-field approximation for the case of cluster formation. Bound states are considered as new species, to be treated on the same level as free particles. A conserving mean-field approach can be formulated by specifying the Feynman diagrams that are taken into account when treating  $A$ -particle cluster propagation [18]. The corresponding  $A$ -particle cluster self-energy is treated to first order in the interaction with the single particles as well as with the  $B$ -particle cluster states in the medium, but with full anti-symmetrization between both clusters  $A$  and  $B$ . We use the notation  $\{A, \nu, P\}$  for the particle number, internal quantum number (including proton number  $Z$ ) and center of mass momentum for the cluster under consideration and  $\{B, \bar{\nu}, \bar{P}\}$  for a cluster of the surrounding medium.

For the  $A$ -particle problem, the effective wave equation reads

$$[E(1) + \dots E(A) - E_{A\nu P}] \psi_{A\nu P}(1 \dots A) + \sum_{1' \dots A'} \sum_{i < j}^A V_{ij}^A(1 \dots A, 1' \dots A') \psi_{A\nu P}(1' \dots A') + \sum_{1' \dots A'} V_{\text{nm}}^{A, \text{mf}}(1 \dots A, 1' \dots A') \psi_{A\nu P}(1' \dots A') = 0, \quad (\text{B1})$$

with  $V_{ij}^A(1 \dots A, 1' \dots A') = V(12, 1'2') \delta_{33'} \dots \delta_{AA'}$ . The effective potential  $V_{\text{nm}}^{A, \text{mf}}(1 \dots A, 1' \dots A')$  describes the influence of the nuclear medium on the cluster bound states and has the form

$$V_{\text{nm}}^{A, \text{mf}}(1 \dots A, 1' \dots A') = \sum_i \Delta(i) \delta_{11'} \dots \delta_{AA'} + \sum_{i, j}' \Delta V_{ij}^A(1 \dots A, 1' \dots A'), \quad (\text{B2})$$

with

$$\begin{aligned} \Delta(1) &= \sum_2 (V(12, 12)_{\text{ex}} \tilde{f}(2) - \sum_{B=2}^{\infty} \sum_{\nu \bar{P}} \sum_{2 \dots B} \sum_{1' \dots B'} f_B(E_{B\nu \bar{P}}) \times \\ &\quad \times \sum_{i < j}^m V_{ij}^B(1 \dots B, 1' \dots B') \psi_{B\nu \bar{P}}(1 \dots B) \psi_{B\nu \bar{P}}^*(1' \dots B'), \\ \Delta V_{12}^A(1 \dots A, 1' \dots A') &= - \left\{ \frac{1}{2} (\tilde{f}(1) + \tilde{f}(1')) V(12, 1'2') + \right. \\ &\quad + \sum_{B=2}^{\infty} \sum_{\nu \bar{P}} \sum_{2 \dots B} \sum_{2' \dots B'} f_B(E_{B\nu \bar{P}}) \sum_j^B V_{1j}^B(1\bar{2}' \dots \bar{B}', 1'\bar{2} \dots \bar{B}) \times \\ &\quad \left. \times \psi_{B\nu \bar{P}}^*(2\bar{2} \dots \bar{B}) \psi_{B\nu \bar{P}}(2'\bar{2}' \dots \bar{B}') \right\} \delta_{33'} \dots \delta_{AA'}, \end{aligned} \quad (\text{B3})$$

$$\tilde{f}(1) = f_1(1) + \sum_{B=2}^{\infty} \sum_{\nu \bar{P}} \sum_{2 \dots B} f_B(E_{B\nu \bar{P}}) |\psi_{B\nu \bar{P}}(1 \dots B)|^2, \quad (\text{B4})$$

where (see Eq. (2); the charge number  $Z$  counts as internal quantum number)

$$f_A(E) = \frac{1}{e^{(E-Z\mu_p-(A-Z)\mu_n)/T} - (-1)^A}. \quad (\text{B5})$$

We note that within the mean-field approximation, the effective potential  $V_{\text{nm}}^{A,\text{mf}}$  remains energy independent, i.e. instantaneous. The quantity  $\tilde{f}(1)$  describes the effective occupation of state 1 due to free and bound states, while exchange is included by the additional terms in  $\Delta V_{12}^A$  and  $\Delta(1)$ , thus accounting for antisymmetrization.

Of course, the self-consistent solution of the cluster in a clustered medium is a rather involved problem which has not been solved until now. In particular, the composition of the medium has to be determined, with energy shifts of the different components (clusters of  $B$  nucleons) in the medium solving the effective wave equation for the  $B$ -nucleon problem.

Two effects have to be considered on the single nucleon level, the quasiparticle energy shift and the Pauli blocking. Phase space is also occupied by clusters as expressed by  $\tilde{f}(1)$ . This effective occupation number is normalized to the total nucleon density. As approximation, a Fermi distribution function that is normalized correspondingly has been used in recent works [4]. Obviously the bound state wave functions and energy eigenvalues as well as the scattering phase shifts become dependent on temperature and density.

### Appendix C: Parametrization of single-nucleon quasiparticle shifts

Different approaches to determine the single-nucleon quasiparticle self-energy shifts are known from the literature. We will not give an exhaustive review but mention only some general features, see also [2]. There are first principle approaches that start from realistic nucleon-nucleon interactions and solve the many-particle problem numerically. Quasiparticle self-energy shifts can also be obtained by different approaches such as the Dirac-Brueckner Hartree-Fock methods or phenomenological density functionals. The latter are based on effective density dependent interactions such as Gogny or Skyrme forces or use relativistic mean-field (RMF) concepts, see [4, 29–31]. Parameter are adjusted to reproduce nuclear bulk properties and properties of nuclei.

There are several relativistic mean-field parametrizations actually used, like TW99 [31], DD [32], DD2 [4], TM1 [7, 33], TMA [6], FSUGold [34] and DDME $\delta$  [35]. We focus on the density dependent DD2 parametrization [4] adjusted to experimental properties of nuclei. In particular, this parametrization predicts reasonable values for the saturation density ( $n_{\text{sat}} = 0.149 \text{ fm}^{-3}$ ), binding energy ( $E/A = -16.02 \text{ MeV}$ ), compressibility ( $K = 242.7 \text{ MeV}$ , what is not far from the experimentally determined value of  $231 \pm 5 \text{ MeV}$  [36]), symmetry energy ( $J = 32.73 \text{ MeV}$ , what fits the experimental value  $31.3 \text{ MeV}$  [37]), and the symmetry slope parameter ( $L = 57.94 \text{ MeV}$  consistent with recent experimental constraints [38]). For neutron stars the model predict a maximum mass of  $2.44 M_{\odot}$ , not in conflict with the largest known mass of  $M = 1.97 \pm 0.04 M_{\odot}$  [39].

For direct use, a parametrization for the DD model [32] was presented in Ref. [4]. We give here an improved parametrization of the DD2 model [4] in form of a Padé approximation. The variables are temperature  $T$ , baryon number density  $n = n_n + n_p$ , and the asymmetry parameter  $\delta = 1 - 2Y_p$  with the total proton fraction  $Y_p = n_p/n$ . The intended relative accuracy in the parameter value range  $T < 20 \text{ MeV}$ ,  $n < 0.16 \text{ fm}^{-3}$  is 0.001.

The spectral function in the RMF approach gives the quasiparticle dispersion relation ( $i = p, n$ , no antiparticles) for the (non-relativistic) single quasiparticle energies

$$e_i(k) = \sqrt{[m_i - S(n, \delta, T)]^2 + k^2} + V_i(n, \delta, T) - m_i. \quad (\text{C1})$$

In the non-relativistic case we have

$$e_i(k) = \frac{k^2}{2[m_i - S(n, \delta, T)]} + V_i(n, \delta, T) - S(n, \delta, T). \quad (\text{C2})$$

With the quasiparticle energies, the chemical potentials  $\mu_i$  follow from solving

$$n_i = \frac{1}{\pi^2} \int_0^{\infty} dk \frac{k^2}{\exp\{[e_i(k) - \mu_i]/T\} + 1}. \quad (\text{C3})$$

The scalar self-energy (identical for neutrons and protons) is approximated as

$$S(n, \delta, T) = s_0(\delta, T) n \frac{1 + s_1(\delta, T) n + s_2(\delta, T) n^2}{1 + s_3(\delta, T) n + s_4(\delta, T) n^2} \quad (\text{C4})$$

with coefficients

$$s_i = s_{i,0} + s_{i,1} T + s_{i,2} \delta^2 + s_{i,3} \delta^4, \quad (\text{C5})$$

densities  $n$  in  $\text{fm}^{-3}$  and temperatures  $T$  as well as the self-energies  $S, V$  in MeV. Parameter values are given in the Table I.

$s_{i,j}$	$i = 0$	$i = 1$	$i = 2$	$i = 3$	$i = 4$
$j = 0$	4463.117	20.56456	15.98022	24.27416	114.5972
$j = 1$	-6.609841	-0.040985	0.866352	-0.074176	1.349746
$j = 2$	-0.170252	-0.339370	-2.020097	-0.542662	2.674353
$j = 3$	4.111559	0.997156	-3.018041	1.196491	0.726793

TABLE I: Coefficients  $s_{i,j}$  for the Padé approximation of the scalar self-energy  $S(n, \delta, T)$ .

The vector self-energy  $V_p(n, \delta, T) = V_n(n, -\delta, T)$  is approximated as

$$V_p(n, \delta, T) = v_0(\delta, T) n \frac{1 + v_1(\delta, T) n + v_2(\delta, T) n^2}{1 + v_3(\delta, T) n + v_4(\delta, T) n^2} \quad (\text{C6})$$

with coefficients

$$v_i = v_{i,0} + v_{i,1} T + v_{i,2} \delta + v_{i,3} \delta^2 \quad (\text{C7})$$

and parameter values given in Table II.

$v_{i,j}$	$i = 0$	$i = 1$	$i = 2$	$i = 3$	$i = 4$
$j = 0$	3403.144	0.662946	10.77796	3.432703	23.01450
$j = 1$	0.000052	-0.006142	0.004432	0.000104	-0.033018
$j = 2$	486.581687	1.140795	-0.802040	1.548693	5.922645
$j = 3$	-2.420361	-0.717645	0.457561	-0.336038	0.050892

TABLE II: Coefficients  $v_{i,j}$  for the Padé approximation of the vector self-energy  $V_p(n, \delta, T)$ .

#### Appendix D: Generating functional approach for the cluster virial expansion

In this Appendix we present instructive examples of approximations to the  $\Phi$  functional on the level of Feynman diagrams to demonstrate the power of this approach. As shown by Baym and Kadanoff [21], any choice of a subset of diagrams for  $\Phi$  defines a selfconsistent approximation, where every Greens function is dressed by its appropriate self-energy obtained by the variation of  $\Phi$ . The advantage of such so-called conserving or  $\Phi$ -derivable approximations is that they satisfy conservation laws and guarantee thermodynamic consistency.

In the past the approach has been applied to a wide variety of many-body problems [23–28] but not yet to the problem of cluster formation in nuclear matter which we are going to discuss here.

In the physical picture the generating functional is represented by the sum of all diagrams that consist of  $A = 2, 3, \dots$  free fermion loops connected by arbitrary numbers of interaction lines. Exchange diagrams have to be added so that the correct symmetry is realized for identical particles. Disconnected diagrams have to be dropped. Only topologically different diagrams are allowed. With the self-energy that is obtained by opening one Green's function line, we can evaluate the density as done in this work. A cluster decomposition for  $\Phi$  is shown in Fig. 3.

A general formalism in the chemical picture is not available at present. The full  $A$ -nucleon (cluster) propagator may be decomposed into a bound and scattering contribution (42), given diagrammatically in Fig. 2. The concept is to consider the bound state part of the  $A$ -particle propagator on the same footing as the single-particle propagator. We illustrate this concept by considering special approximations that have been used in the present work. The relevant diagrams are selected by construction.

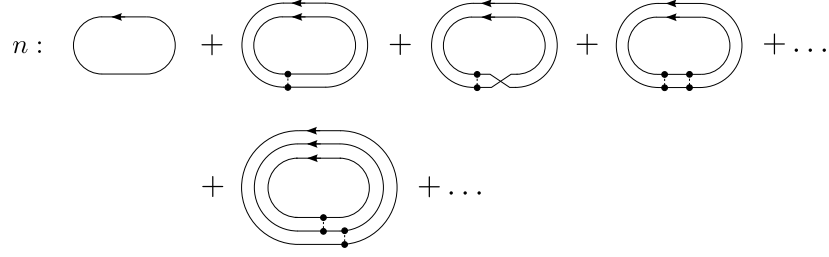


FIG. 3: Cluster decomposition of the generating functional  $\Phi$ . Some contributions for  $A = 2, 3$  are shown explicitly, the ladder sum has to be completed considering an arbitrary number of interaction lines. The single particle loop has been added to represent the ideal part of the density.

The ideal gas of nucleons follows from the first diagram of Fig. 3. The Hartree-Fock (HF) contribution to the second virial coefficient follows from the second diagram and the corresponding exchange term. The sum of all ladder diagrams with  $A = 2$  yields a Bethe-Salpeter equation that contains a scattering part and eventually a bound state part. For  $A = 2$ , this binary approximation for  $\Phi$  generates the standard Beth-Uhlenbeck formula. In the chemical picture, we obtain the nuclear statistical equilibrium (NSE) supplementing the single nucleon propagator (first diagram of Fig. 3) by the propagator of bound states, see Fig. 4.

$$n^{\text{NSE}} : \sum_A \text{loop with } A \text{ interaction lines}$$

FIG. 4: Generating functional for the nuclear statistical equilibrium (NSE).

Within the single-nucleon approach, the corrections in lowest order of the interaction are given by the Hartree-Fock approximation. The corresponding Hartree-Fock approximation  $\Phi^{\text{HF}}$  (as the simplest version of a quasiparticle

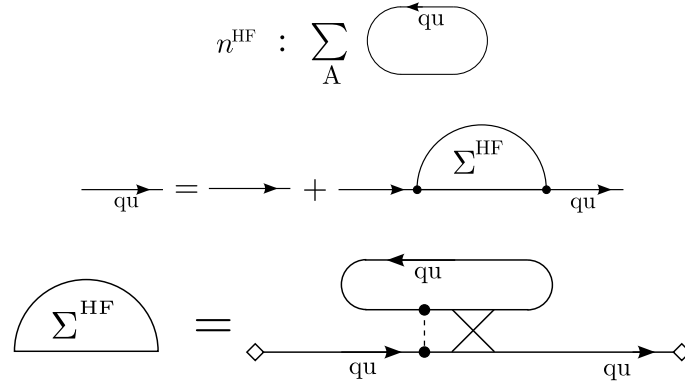


FIG. 5: Hartree-Fock approximation for the generating functional  $\Phi^{\text{qu}}$ . The dotted line is the interaction. The crosses lines denote antisymmetrization. The diamonds at the endpoints of Green functions denote amputation (multiplication with the inverse).

approximation) is shown in Fig. 5. The dotted line represents the interaction. The crossed lines denote antisymmetrization. Note that bookkeeping has to be respected. Diagrams that are included in  $\Phi^{\text{HF}}$  have to be subtracted from other groups. For instance, the first order diagrams of the ladder sum in Fig. 3 (the second and third diagram) have to be subtracted.

Turning to larger clusters, we can also define a quasiparticle propagator according to Eq. (A6). The presentation by diagrams using the  $A$ -cluster self-energy is given in Fig. 6. Then,  $\Phi^{\text{HF}}$  is completed according to the chemical picture by the cluster mean-field approximation for the generating function  $\Phi^{\text{CMF}}$  shown in Fig. 6. This approximation contains the cluster mean-field as described in App. B.



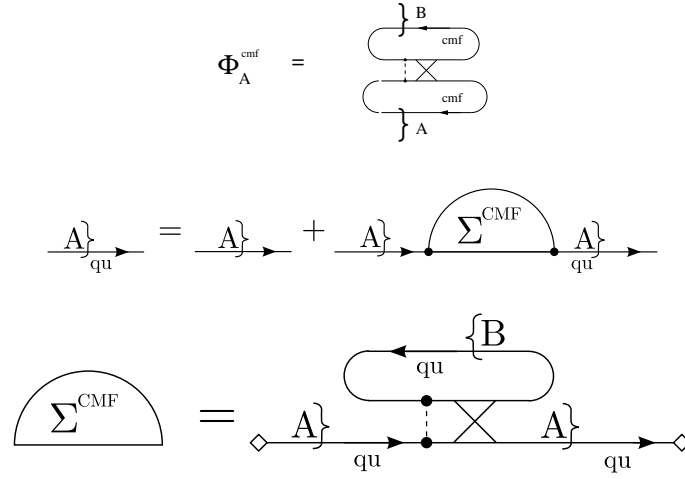


FIG. 6: Quasiparticle propagator for cluster with cluster mean-field self-energy. The crossed lines means the full antisymmetrization between the clusters A and B. The diamonds at the endpoints of Green functions denote amputation (multiplication with the inverse).

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- [41] Note that the interaction in nuclear systems is strong. However, the perturbation expansion is performed with respect to the imaginary part of the self-energy that is assumed to be small. Most of the interaction is already taken into account in the self-consistent determination of the quasiparticle energies. With increasing density, the Fermi energy will dominate the potential energy so that the correlations are suppressed. A quasiparticle description can be used to calculate the nuclear structure.